APPENDIX O

DEFINITIONS OF FACTORS AFFECTING ENVIRONMENTAL FATE AND TRANSPORT
OF CHEMICALS

APPENDIX O
DEFINITIONS OF FACTORS AFFECTING ENVIRONMENTAL
FATE AND TRANSPORT OF CHEMICALS

As stated in Section 5.0, mobility and persistence are the two major characteristics affecting the fate and transport of a chemical in environmental media. Definitions of the factors affecting environmental fate and transport of chemicals are provided below.

Solubility is the measure of a chemical's ability to dissolve in a solvent and is expressed in units of chemical mass per unit volume of solvent (e.g., ug/L or mg/L). Aqueous solubility is an important determinant of chemical concentration and residence time in water. Highly soluble chemicals readily dissolve in water and remain in solution, whereas chemicals having low solubility tend to be unstable in solution. In addition, solubility often predicts the ease with which chemicals are leached from wastes and soils.

Sorption (adsorption/desorption) is the reversible binding of a chemical to a solid matrix. Both soluble nonpolar and insoluble chemicals usually adsorb strongly to sediments, suspended solids, and soils. Adsorption of these compounds to a solid phase limits the fraction available for other fate processes such as volatilization and hydrolysis. Although adsorption is generally modeled as a fully reversible process, there is evidence in published literature that there is a partially irreversible component related to the length of time that the material has been adsorbed. Generally, the less polar and less soluble the chemical, the greater the adsorption to the solid phase (i.e., soils, sediments, and suspended solids). Partition coefficients, which are important measures of sorptive characteristics, define the relative concentration of a given chemical in two phases or matrices.

Partition coefficients are expressed as concentration ratios; higher values indicate a greater tendency to associate with the non-aqueous phase. Partition coefficients useful in describing the environmental behavior of a compound include K_{ow}, K_d, and K_{oc}, and are defined:

- K_{ow}: The octanol-water partition coefficient is the ratio of chemical concentration in octanol (an organic solvent) to that in water at steady-state conditions. Octanol serves as a surrogate for lipids or other organic phases. High K_{ow} values indicate an increased tendency of a compound to sorb to organic matter in soils or sediments, and are associated with elevated bioconcentration factors in biota.

- K_d: The soil-water partition coefficient is the ratio of chemical concentration in aqueous and solid phases at steady-state conditions (usually applied to inorganic species). Small K_d values indicate the chemicals are highly leachable and are not likely to be bound to soil particles. High K_d values indicate a propensity to sorb onto soil particles.

- K_{oc}: The organic carbon partition coefficient is the K_d normalized to the concentration of organic carbon in the soil, since in many surface soils, the soil organic carbon is the dominant sorbent for hydrophobic organic compounds (Karickoff, et. al., 1979). High K_{oc} values usually indicate a high tendency of a compound to sorb to organic matter in soils or sediments.

Volatilization describes the movement of a chemical from the surface of a liquid or solid matrix to a gas or vapor phase. Only the neutral (uncharged) form of compounds can volatilize. Therefore, the fraction of the compound in the uncharged form should be calculated using pKa (acids) or pKb (bases) under site pH conditions. Volatilization is calculated from the equilibrium vapor pressure, which is a measure of chemical solubility in air (when the initial chemical concentration is in the liquid phase). Volatilization losses to air are correlated with chemical concentration, molecular weight, solubility, and ambient temperature. Volatilization is a particularly important environmental fate process for nonpolar chemicals having low aqueous solubility. Volatilization from the liquid phase is measured by the Henry's Law Constant, which can be expressed as the quotient of the chemical's vapor pressure to its solubility at a specific temperature. Lyman et al. (1982) described compounds as readily, significantly, or limitedly volatilized based on the values of their Henry's Law Constants. These values in atm-m^3/mol are $\geq 10^{-3}$, 10^{-3} to 10^{-5}, and $< 10^{-5}$, respectively.

Bioconcentration is the accumulation of a chemical directly from the exposure medium or source material into an organism. For example, plants or animals associated with exposures to ambient water, soil, air, or sediment may bioconcentrate chemicals from these media via ingestion and/or direct absorption through the organisms' exposed surfaces. After entering the organism, contaminants may become concentrated within specific tissues as the result of metabolic pathways that yield the same chemical for storage within the organism, or via direct deposition of the contaminant in certain tissues without being metabolized and/or excreted.

Bioaccumulation is the accumulation and transport of a chemical from a specific media through both the food chain and bioconcentration. The potential for bioaccumulation may be quantified by equilibrium bioconcentration factors (BCFs), which define the ratio of a chemical concentration in animal or plant tissue to the concentrations of the same chemical in the environmental media of contact. Organic chemicals with high BCFs (such as pesticides, PCBs, etc.) are typically insoluble and lipophilic (nonpolar) and, thus, tend to reside in animal fat tissue. Some heavy metals may also bioaccumulate. Literature values of BCFs most commonly pertain to fish species.

Biotransformation/biodegradation is the metabolic transformation of complex molecules into other compounds by microorganisms. Products of biotransformation/biodegradation may or may not be toxic to other organisms, and these products may undergo further biotransformation/biodegradation. Biological transformation includes a variety of enzyme-catalyzed reactions such as oxidation and reduction.

Oxidation is a chemical reaction which involves the removal of electrons from an element or compound. Conversely, electrons are added to chemical substrates in **reduction** reactions. Both oxidation and reduction reactions are environmentally significant in that they influence the mobility and fate of chemicals in environmental matrices. Oxidized and reduced forms of the same element or compound may also have totally different chemical, ecological, and toxicological properties. For example, hexavalent chromium (i.e. Cr(+6)) is an oxidized valence state of chromium that is generally highly toxic, whereas trivalent chromium (i.e., Cr(+3)) is a reduced form of chromium that is generally less toxic. Oxidation-reduction reactions are commonly referred to as "redox" reactions.

Hydrolysis is the reaction of a chemical with water or with hydrogen (H+) or hydroxyl (OH-) ions. These components of water interact with, or attack, sites of a chemical resulting in subsequent breakdown or modification in the environment. The extent of chemical hydrolytic reactivity depends on both pH (acidity/alkalinity) and molecular structure of the specific chemical.

Photolysis is a chemical decomposition process induced by radiant energy (sunlight). The rate of loss of a chemical from photochemical reactions depends on both its molecular structure and the proximity and character (i.e., wavelength) of the light source, and the presence of other reactive compounds.